

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.98e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.61e-01

Confidence level: 7.61e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Cycloate</div> <div>Measured: 3.95e-04</div> <div>Predicted: 2.98e-04</div>	<div>Image not found</div> <div>Pebulate</div> <div>Measured: 4.92e-04</div> <div>Predicted: 4.82e-04</div>	<div>Image not found</div> <div>Butylate</div> <div>Measured: 2.07e-04</div> <div>Predicted: 3.42e-04</div>
<div>Image not found</div> <div>Vernolate</div> <div>Measured: 4.43e-04</div> <div>Predicted: 4.86e-04</div>	<div>Image not found</div> <div>Diallate</div> <div>Measured: 5.18e-05</div> <div>Predicted: 9.66e-05</div>	